determination of the mechanism of the reactions of $FeRu(CO)_6(\alpha$-diimine) complexes with molecular hydrogen (Zoet *et al.*, 1989); these reactions in the presence of an additional ligand led to the formation of the title compound. The synthesis of this compound will be presented in a separate paper together with its chemical and spectroscopic properties (Kraakman, Goubitz, Numan & Vrieze, 1991).

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Structure of α-Cyclopiazonic Acid

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Abstract. $C_{20}H_{20}N_2O_3$, $M_r = 336.1$, tetragonal, $P4_32_12$, $a = 10.406\ (1)$, $c = 61.549\ (14)$ Å, $V = 6664\ (2)$ Å^3, $Z = 16$, $D_x = 1.34$ g cm^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 6.20$ cm^{-1}, $F(000) = 2832$, $T = 298$ K, final $wR = 0.064$ ($R = 0.077$) for 3357 reflections and 470 variable parameters. α-Cyclopiazonic acid is the main toxic principle of the strain CSIR 1082 (ATCC 36064 or NRRL 3523) of *Penicillium griseofulvum* Dierckx. The molecule crystallizes as an *exo*-enol rather than the *endo*-enol tautomer as suggested [Holzapfel (1968). *Tetrahedron*, **24**, 2101–2119], and the *exo*-cyclic enolic moieties have different orientations in the two molecules in the asymmetric unit.

Experimental. The title compound was obtained as described previously, and isolated as pale brown octahedral crystals from MeOH/$CHCl_3$ (m.p. 522–524 K) (Holzapfel, 1968). Crystal $0.17 \times 0.19 \times 0.24$ mm, Philips PW 1100 diffractometer, graphite monochromator, unit cell from 25 reflections ($17 < \theta < 23°$), 5924 reflections for $5 < \theta < 60°$ in the range $0 < h < 11$, $0 < k < 11$, $0 < l < 69$ using ω–2θ scans, peak scan width 0.40°, scan speed 0.96° min^{-1}, backgrounds not measured but assumed isotropic and calculated as a function of θ from the counts of systematically absent reflections. Three standard reflections measured every 130 reflections. Lp correction applied, no decay or absorption corrections. 3357 unique reflections with $F > 2\sigma(F)$ used, structure solved using *SHELXS*86 (Sheldrick, 1986), all hydrogen atoms placed in calculated positions (C—H 1.08 Å, H—C—H 109.5°, C=C—H 120.0°), least-squares refinement on F using *SHELX*76 (Sheldrick, 1976), $\sigma^{-2}(F)$ weights, all non-hydrogen atoms anisotropic, hydrogen atoms isotropic and constrained to ride upon their associated heavy atoms with a common thermal parameter that refined to $U_{iso} = 0.105\ (4)$ Å^2. Final $wR = 0.064$, $R = 0.077$, maximum positional shift/e.s.d. less than 0.7, residual electron density = 0.40 e Å^{-3}. Scattering factors from *SHELX*76. Table 1 gives the atom parameters.* Fig. 1 shows the molecular structure and the numbering scheme of molecule *A*, drawn by *ORTEP* (Johnson, 1965). For the second molecule *B* the positions of O2 and C18 in Fig. 1 should be interchanged. Table 2 gives selected bond distances and bond angles.

Related literature. The existence in solution of the *exo*-cyclic enol tautomer is also indicated in NMR studies of related compounds (Nolte, Steyn & Wessels, 1980; Steyn & Wessels, 1978).

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* Lists of structure factors, anisotropic thermal parameters, H-atom parameters and a complete list of bond lengths and angles have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 54501 (22 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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Table 1. *Fractional coordinates* ($\times 10^4$) *and equivalent isotropic thermal factors* ($\times 10^3$ Å^2) *for α-cyclopiazonic acid*

$U_{eq} = \frac{1}{3}\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq}
N1*A*	3016 (6)	86 (5)	9126 (1)	69 (2)
C1*A*	3841 (7)	1089 (6)	9073 (1)	62 (2)
C2*A*	3123 (7)	2132 (6)	9017 (1)	56 (2)
C3*A*	3468 (6)	3485 (6)	8948 (1)	55 (2)
C4*A*	4437 (6)	4147 (6)	9107 (1)	51 (2)
C5*A*	5730 (6)	4557 (7)	9018 (1)	59 (2)
C6*A*	5817 (7)	5919 (7)	9040 (1)	57 (2)
C7*A*	4593 (6)	6405 (7)	9125 (1)	54 (2)
N2*A*	3822 (5)	5382 (5)	9165 (1)	52 (1)
C8*A*	2403 (6)	5239 (6)	9154 (1)	54 (2)
C9*A*	2286 (6)	4444 (6)	8946 (1)	55 (2)
C10*A*	953 (6)	3823 (6)	8903 (1)	62 (2)
C11*A*	725 (7)	2505 (6)	8996 (1)	57 (2)
C12*A*	−449 (7)	1960 (8)	9037 (1)	75 (2)
C13*A*	−515 (8)	641 (8)	9104 (1)	81 (2)
C14*A*	573 (8)	−103 (7)	9138 (1)	73 (2)
C15*A*	1740 (8)	511 (7)	9105 (1)	61 (2)
C16*A*	1825 (7)	1796 (6)	9037 (1)	51 (2)
C17*A*	6833 (8)	6654 (8)	8986 (1)	75 (2)
C18*A*	7977 (6)	6151 (9)	8892 (1)	98 (3)
C19*A*	1942 (6)	4537 (6)	9360 (1)	66 (2)
C20*A*	1721 (7)	6533 (6)	9128 (1)	68 (2)
O1*A*	6531 (5)	3771 (5)	8947 (1)	85 (1)
O2*A*	6763 (6)	7997 (6)	9016 (1)	119 (2)
O3*A*	4334 (4)	7552 (4)	9151 (1)	65 (1)
N1*B*	4884 (5)	−5635 (5)	9690 (1)	58 (1)
C1*B*	4211 (6)	−4590 (6)	9778 (1)	59 (2)
C2*B*	4928 (6)	−3503 (6)	9755 (1)	49 (2)
C3*B*	4749 (6)	−2143 (5)	9822 (1)	53 (2)
C4*B*	4001 (6)	−1302 (6)	9662 (1)	53 (2)
C5*B*	2550 (7)	−1198 (7)	9674 (1)	57 (2)
C6*B*	2267 (7)	155 (7)	9695 (1)	59 (2)
C7*B*	3443 (7)	857 (7)	9723 (1)	65 (2)
N2*B*	4451 (5)	10 (5)	9705 (1)	59 (1)
C8*B*	5600 (7)	37 (6)	9839 (1)	66 (2)
C9*B*	6049 (6)	−1402 (6)	9833 (1)	60 (2)
C10*B*	6909 (7)	−1671 (6)	9631 (1)	63 (2)
C11*B*	7103 (6)	−3086 (6)	9591 (1)	57 (2)
C12*B*	8152 (7)	−3676 (7)	9493 (1)	71 (2)
C13*B*	8115 (7)	−5015 (7)	9455 (1)	70 (2)
C14*B*	7102 (7)	−5798 (7)	9508 (1)	66 (2)
C15*B*	6059 (7)	−5192 (6)	9613 (1)	55 (2)
C16*B*	6078 (6)	−3874 (6)	9650 (1)	52 (2)
C17*B*	1043 (8)	650 (8)	9700 (1)	80 (2)
C18*B*	776 (11)	1963 (7)	9713 (2)	143 (4)
C19*B*	5260 (8)	374 (7)	10082 (1)	81 (2)
C20*B*	6599 (7)	1004 (7)	9759 (1)	92 (2)
O1*B*	1783 (4)	−2105 (4)	9665 (1)	79 (1)
O2*B*	−23 (5)	−215 (7)	9694 (1)	128 (2)
O3*B*	3552 (5)	2018 (5)	9759 (1)	90 (2)

Table 2. *Selected bond distances* (Å) *and bond angles* (°) *for α-cyclopiazonic acid*

	A	*B*
C5—C6	1.427 (9)	1.444 (8)
C6—C7	1.467 (8)	1.435 (8)
C6—C17	1.347 (9)	1.374 (9)
C17—O2	1.411 (8)	1.429 (9)
C17—C18	1.422 (9)	1.397 (9)
C5—C6—C7	108.7 (6)	109.4 (6)
C5—C6—C17	126.2 (7)	123.8 (7)
C7—C6—C17	125.1 (7)	126.7 (7)
C6—C17—O2	119.3 (8)	118.9 (7)
C6—C17—C18	123.2 (8)	123.5 (9)
O2—C17—C18	117.5 (8)	117.6 (8)

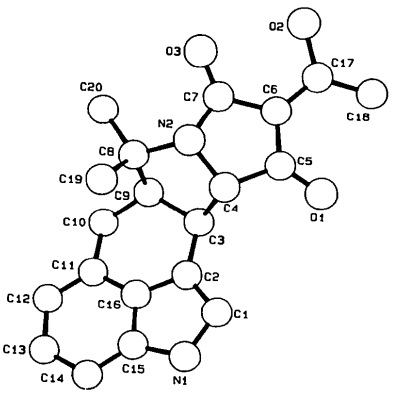

Fig. 1. Perspective view with atomic numbering scheme.

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Structure of Citreohybridone A

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Abstract. $C_{30}H_{38}O_9$, $M_r = 542.6$, orthorhombic, $P2_12_12_1$, $a = 13.119$ (1), $b = 22.204$ (3), $c = 9.868$ (1) Å, $V = 2874.5$ (5) Å^3, $Z = 4$, $D_x = 1.25$ Mg m^{-3}, λ(Mo $K\alpha$) = 0.71073 Å, $\mu = 0.086$ mm^{-1}, $F(000) = 1160$, $T = 297$ K, $R = 0.067$ for 1914 observed unique reflections. The relative structure of a new cytotoxic substance against HeLa cells has been determined by single-crystal X-ray

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